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McStas event logger: Definition and Applications

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1. Abstract

Functionality is added to the McStas neutron ray-tracing code, which allows individual neutron states before and after a scattering to be temporarily stored, and analysed. This logging mechanism has multiple uses, including studies of longitudinal intensity loss in neutron guides and guide coating design optimisations. Furthermore, the logging method enables the cold/thermal neutron induced gamma background along the guide to be calculated from the un-reflected neutron, using a recently developed MCNPX-McStas interface.

Keywords: Neutron, Transport, Simulation, MCNPX, McStas, Interface, neutron optics, guide, dose.

2. Introduction

When constructing a neutron scattering facility, a major problem faced is the design of neutron guides and the surrounding shielding. For many years, the design of neutron guides has been governed by the rather simple design goal of transporting as many neutrons as possible to the sample position. Development in sputtering techniques have in recent years made neutron guides of high m -values available commercially, yet at a very high price. Thus it is of interest to evaluate how and where to use high m -value guides and where a less pricy guide section might be used without significantly harming performance[1]. Furthermore, depending on the experiment, the higher divergence neutrons that may be transported using the high m -values guides may be of little scientific value. In addition, the value of the higher divergent neutrons should also be offset by the amount of background radiation that will infallibly be generated in the guide walls by imperfect neutron reflections[2]. Such an offset may even render transport of higher divergence neutrons harmful to the experiment.

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These issues may be seen as different views of the same wish to tailor the neutron guide design (including shielding) to the particular source and instrument in question. For instance it is advantageous to design guides such that background is primarily generated at locations where it is less harmful to the instrument signal, and indeed to the neutron signal of neighbouring instruments.

Shielding considerations is another aspect where absorbed neutrons are of interest. Shielding must be adequate for the obvious reason that humans outside the shielding should not irradiated, nor should neighbouring instruments be affected by escaping neutrons.

The fabrication cost of a neutron guide, whilst substantial, is frequently a minor fraction of the cost of an instrument project. The construction of good shielding for modern spallation source instruments, on the other hand, is a major cost driver.

Monte Carlo tools are very well suited for neutron instrumentation calculations due to the independent nature of neutron particles in a beam. Several tools are available[3, 4, 5, 6, 7] focused on neutron instrumentation calculations handling epi-thermal to cold neutron beams. Other software packages are available for high to moderate energy neutronics[8, 9, 10], but are not practical for calculations involving transport over long distances and/or coherent scattering processes.

The intensity lost or deposited in the guide walls is neglected in the neutron instrumentation codes. This work aims at remedying this. We have chosen to extend the neutron ray tracing package McStas[11] with functionality allowing users to analyse scatter events using their accustomed work flows, for instance by injecting the lost intensity into MCNPX-calculations aimed at evaluating background levels (of e.g. gamma-radiation) in the vicinity of the neutron guide.

In the following we will first present the working principle of the McStas addition, followed by three use-cases where in turn the deposited intensity, the coating m -value characteristics, and the generated gamma-background is examined for a simple but realistic neutron guide.

3. Functionality

Software was written enabling the details of any interaction of a neutron with a McStas[3, 4, 12, 13] component to be temporarily stored and analysed. Based on a user assigned component, the full neutron parameter state (position, velocity, spin, time & weight) before and after any interaction occurring in the component is stored in memory. When the neutron exits the component, the logging mechanism is disabled and the user can iterate through the intermediate neutron interactions which took place and perform detailed studies (examples are given below). Once complete the intermediate structures are flushed to prevent memory built-up and the neutron proceeds the instrument simulation unaltered. A visualisation of a guide and the logging utility in operation is shown in Figure 1. At the points where a neutron ray hits the guide wall, the un-reflected fraction is emitted as a secondary ray, propagated to an object surrounding the guide where it may be detected and monitored.

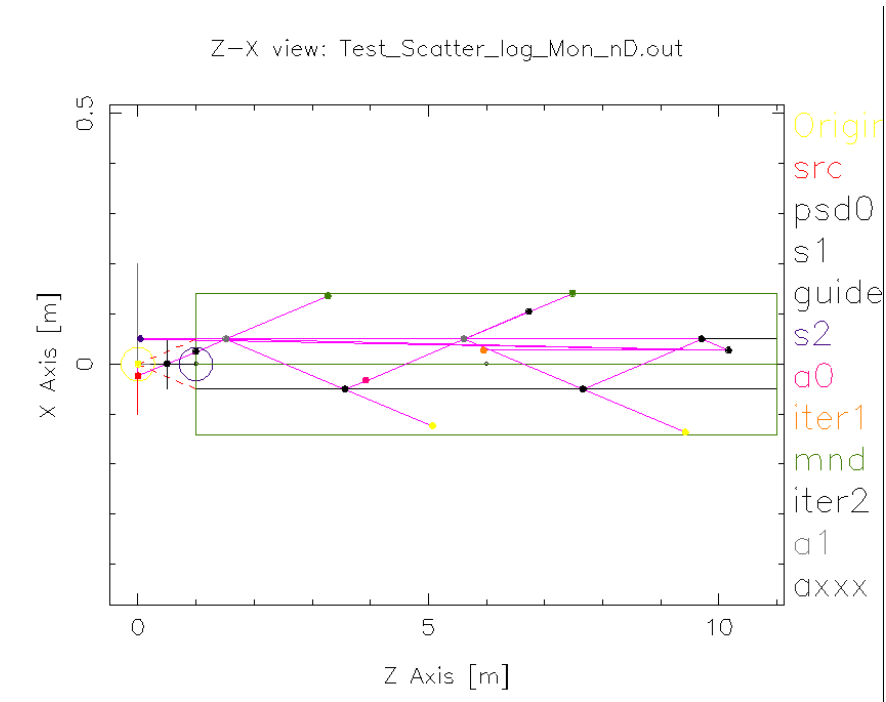


Figure 1: Basic guide geometry - from McStas' *mcdisplay*. Also shown in the figure is an example neutron trajectory. At each encounter with the guide wall, both the reflected and un-reflected neutron ray is stored and both trajectories are visualised. The un-reflected ray is allowed to propagate to a monitor object surrounding the guide where it is detected.

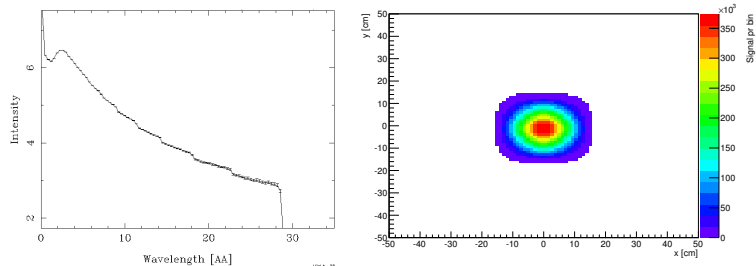


Figure 2: Spectrum(left) and beam-profile(right) of the neutron source on which the examples are based. Measured at the guide entrance. The small discontinuities apparent in the spectrum are due that the spectrum is generated with MCNPX using energy bins rather than bins of wavelength (i.e. the trend across a given energy bin is unaccounted for - the spectrum shows the (lack of) validity of this approximation).

4. Examples

For illustration purposes, consider neutron guides under consideration to be built at the future European Spallation Source (ESS):

- 50 m straight and curved guides (radius of curvature = 1500 m)
- m -value = 3
- Size of neutron channel: $4 \times 4 \text{ cm}^2$
- Preliminary ESS source spectrum and moderator geometry

The moderator is $12 \times 12 \text{ cm}^2$ and is placed at a distance of 2 m from the guide entrance. Combined with the fact that the beam has a divergence of 2.5° (flat in $\cos(\Theta)$), this means that significantly more than the neutron channel opening is illuminated by neutrons. This over-illumination will play a role for Example 3 below. Figure 2 shows the beam-profile/footprint and energy spectrum at the entrance of the guide.

4.1. Example 1: Neutron trace

Figure 3 shows the result of a simple McStas simulation of the guide, where the logging capability is used to histogramize, at runtime, where neutron intensity is lost due to imperfections of the guide mirrors ($m = 3$).

As expected, the majority of the intensity is lost in the first part of the guide. Further, we find that neutron beams in curved guides lose more intensity in the latter part of the guide, compared to beams in straight guides. These are simply geometrical effects, reflecting that in the first part of the guide, neutrons may hit the wall at higher angles of incidence than further downstream. In the case of a curved guide, high energy neutrons on straight trajectories are also lost, which accounts for the higher loss in the curved guide case. Qualitatively this is neither new, nor surprising, but serves as a sanity check of the developed procedure and shows that it yields a quantitative handle on the problem of appropriately shielding neutron guides, even for guides with more complex geometries.

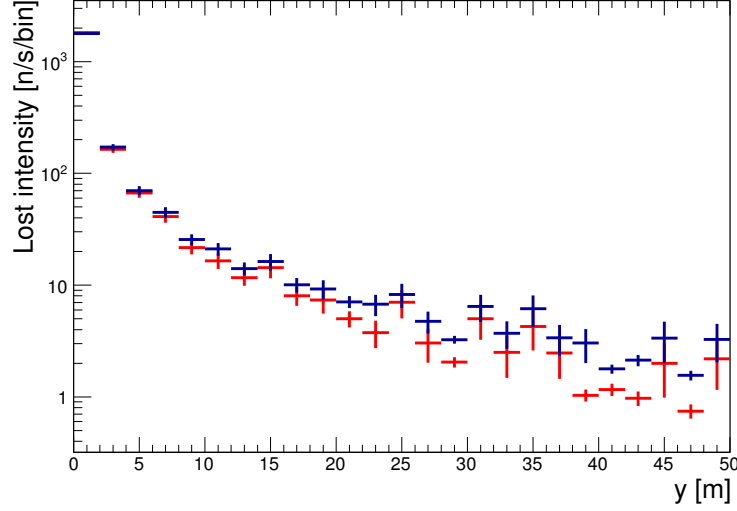


Figure 3: Histogram showing the lost neutron intensity along straight (red) and curved (blue) guides as described in the text.

4.2. Example 2: Supermirror requirements along guide

In addition to simply trace the neutron interactions in a guide as discussed in the above example, one can also exploit the fact that at each interaction, one has access to *all* the parameters describing a neutron state, including its velocity vector. To this end, consider for example the use-case of guide coating design. Guides, and especially high m -value long guides, are expensive and their cost is depends strongly on the reflection requirements. It is therefore beneficial to, as much as possible, choose guide sections with low reflectivity requirements or equivalently low m -value. The minimum m -value required to reflect a given neutron is defined as the following [13]:

$$m_{min} = 2 \cdot k \cdot \sin(\theta) / 0.0219 \quad (1)$$

where θ is the inclination angle between the neutron and the guide wall and k is the scattering vector¹. Using the logging techniques, m_{min} along the guide is shown for the 'first', 'second', 'third' and 'all' reflection in Figure 4, as a function of y along guide. The line-of-sight is lost for the first time at at 22 m, and for the second time at 44 m which explains the unfilled phase-space regions of the figures corresponding to the first and second reflections. The guide itself has an

¹For our purposes, it is of little importance that in practice there is a smooth transition between reflection and absorption. Also we assume the reflectivity plateau to 100% reflecting, which is also an approximation.

$m = 3$ coating. Thus, intensity above $m = 3$ in either of the plots in Figure 4 will predominantly be lost and not transported to be reflected again.

Using this kind of data, it is conceivable to tailor the guide coating design to loose the most neutron intensity where it is least inconvenient in terms of radiation shielding and interference with neighbouring instruments.

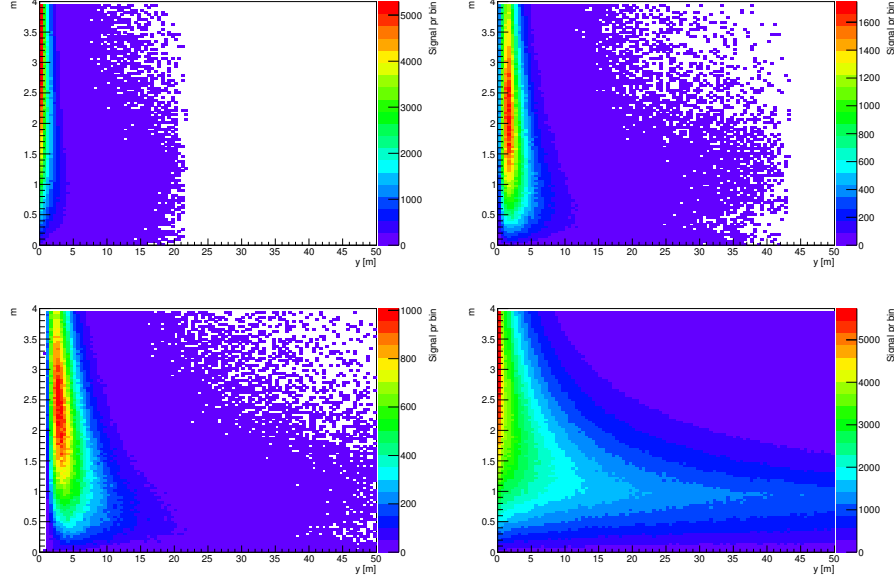


Figure 4: Histograms showing the minimum m -value required for a reflection, as a function of y along guide in a simulation of the curved guide described in Section 4. The color scale indicates the bin intensity. Note that the simulation was carried out using a $m = 3$ guide, which is seen to cause significant intensity loss in the beginning of the guide. Note that no 'first' reflections occur beyond $y = 22$ m where direct line of sight is lost, and no 'second' reflections occur beyond $y = 44$ m.

4.3. Example 3: Coupling to MCNPX

In addition to tracking the (un-)scattered neutrons, the developed software can be used to derive quantities related to the radiation caused by a neutron beam along the guide. In standard McStas simulation, a typical scattering event results in a directional change of the neutron associated with a weight difference which, according to McStas, accounts for the imperfections of the mirror. Normally, the un-reflected neutrons are simply discarded - i.e. the leaking weight is ignored, but by using a combination of the event logging technique described in the present paper as well as recently developed methods to interface McStas and MCNPX[14] (which is a general Monte Carlo transport code, capable of accurately describing incoherent scattering [8, 15]), the simulation and neutron transport can proceed in the guide walls aiming at determining the radiation caused by the un-reflected neutrons.

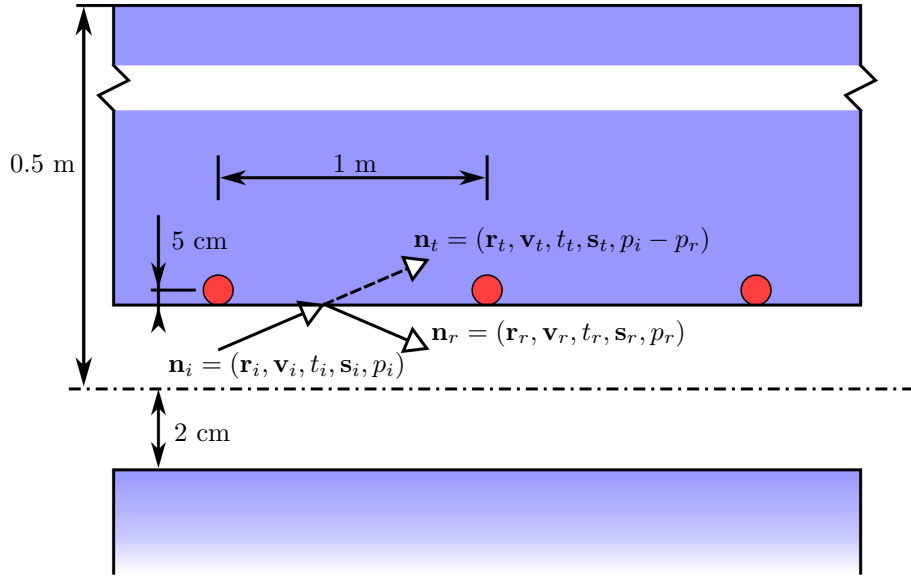


Figure 5: Sketch of the experimental configuration used in Section 4.3. Neutrons travel through a $4 \times 4 \text{ cm}^2$ guide which is situated centrally in a $1 \text{ m} \times 1 \text{ m}$ steel housing (blue). The dose-rate is measured in spherical detectors (red) situated 5 cm inside the steel blocks spaced 1 m apart. Also indicated are a neutron ray, \mathbf{n}_i , encountering the guide wall, a reflected ray, \mathbf{n}_r , and a transmitted ray, \mathbf{n}_t , which is computed from the logged states. The latter is injected into MCNPX. Not that teh sketch is out of scale.

Consider again neutrons interacting with the two 50 m example guides. In the intermediate analysis of the scattering events of a given neutron, each scattering event instantiates the software interface to MCNPX with the incoming neutron parameters and the reduced weight as input parameters. By this the leaking neutron states are stored for offline use.

In the post-processing a MCNPX simulation is launched based on the same geometry model, and the stored event file. A example visualisation of the interactions taking place in MCNPX is shown in Figure 6.

Of special interest is the radiation dose rate in the vicinity of the guide in a realistic shielding scenario (Figure 5). Assuming 1 m steel guide housing the dose rate at 5 cm from the guide wall (i.e. in the steel, close to the neutron channel) along the guide is shown in Figure 7. The dose-rate in the first ~ 10 m is partly due to un-reflected neutrons from within the guide, but mainly due to neutrons that missed the neutron channel and entered the steel shielding at the end of the guide. In the curved guide, line-of-sight from the moderator surface is lost at 22 m explaining the drop in neutron dose rate at this y -value. Even at this significant distance from the guide opening, the photon dose rate is still dominated by (n, γ) reactions at the guide opening and thus the drop in neutrons converting (see where line-of-sight is lost at $y = 22$ m) has no apparent effect on the photon dose rate. To avoid this masking, consider Figure 8 which shows the same as Figure 7 but only for the select wavelength range 0.5 Å–1.0 Å. Clearly the curves show the same trends as expected since in this limited wavelength span the photons should be dominantly generated by (n, γ) processes within the guide. Obviously this is a somewhat idealised situation - in a more realistic scenario a velocity selector could be introduced and simulated. However the scope here is mainly to illustrate capabilities and to validate the developed software and therefore a more realistic rejection of high-energy neutrons has been omitted for reasons of simplicity.



Figure 6: Neutron (red) and photon (green) trajectories, caused by a few example neutrons interacting with an example guide (blue, see Figure 1). The simulation of the unreflected neutrons is carried out by MCNPX and illustrated using *Vised*[16].

5. Usage

To enable McStas logging capabilities, McStas release 2.0 is required. The components are available for download from the McStas homepage[11] (GPL 2 license). The documentation on usage can be retrieved in `html` format using the standard McStas documentation utility: `mcdoc`. For coupling to MCNPX a personal license is required. Events are read in/out

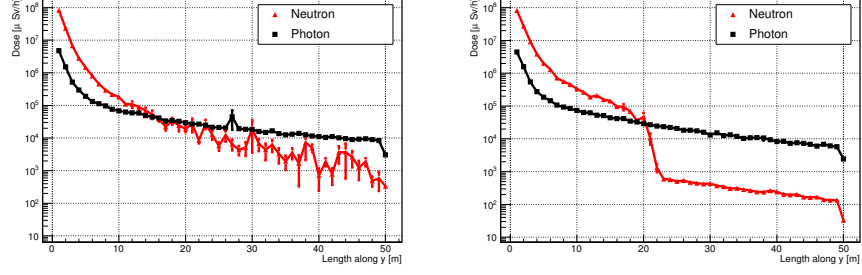


Figure 7: Histograms showing the dose rate along the straight (left) and curved (right) described in Section 4. Energy- and particle dependent conversion factors have been applied when converting from fluence to effective dose in accordance with Swedish radiation protection authorities[17, 18].

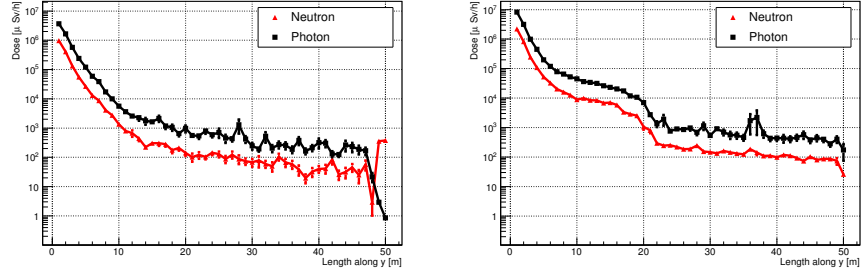


Figure 8: Histograms showing the dose rate along the straight (left) and curved (right) example guides described in section 4. Only neutrons in the wavelength range: 0.5 Å- 1.0 Å are accounted for. Energy- and particle dependent conversion factors have been applied when converting from fluence to effective dose in accordance with Swedish radiation protection authorities[17, 18].

using `Virtual_mcnp_ss_input/Virtual_mcnp_ss_output` components respectively.

6. Conclusions and prospects

As the examples discussed above show, the developed tool is very useful for detailed studies of neutrons interacting with guides. When the ESS is fully operational it is planned to serve 22 instruments utilising a number of different guide configurations. It is envisioned to use the methods outlined here individually for each guide geometry, since the method can only be done with confidence on an instrument to instrument basis. Foreseen additional applications include the simulation of expected background at the sample and/or instrument position, originating from gammas from unreflected neutrons and/or activation.

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